

Striped superconductors in the extended Hubbard model.

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We present a minimal model of a doped Mott insulator that simultaneously supports antiferromagnetic stripes and d -wave superconductivity. We explore the implications for the global phase diagram of the superconducting cuprates. At the unrestricted mean-field level, the various phases of the cuprates, including weak and strong pseudogap phases, and two different types of superconductivity in the underdoped and the overdoped regimes, find a natural interpretation. We argue that on the underdoped side, the superconductor is intrinsically inhomogeneous – striped coexistence of superconductivity and magnetism – and global phase coherence is achieved through Josephson-like coupling of the superconducting stripes. On the overdoped side, the state is overall homogeneous and the superconductivity is of the classical BCS type.

Experimental evidence increasingly suggests that microscopic inhomogeneous “stripe” states are ubiquitous in the doped cuprates, as well as in other complex electronic materials [1]. Nanoscale stripe morphologies have been inferred in YBCO and LSCO from neutron scattering and angle resolved photoemission experiments. In the superconducting phase, the stripes appear to coexist with superconductivity in a range of dopings without destroying the global phase coherence. The main issue that we address in this Letter is the nature of the superconducting state in the presence of stripes.

Inhomogeneous quantum states in non-superconducting lattice models are no less common than they are in the experiments. Many lattice models possessing antiferromagnetic (AF) ground states at half-filling, when doped away from that filling develop stripes at the unrestricted mean-field (MF) level [2–5]. Exact solutions may lead to fluctuations that introduce dynamics into the MF solutions, but are expected to preserve the qualitative features. The lower the spatial dimension the more important the quantum fluctuations are and, sometimes, MF solutions do not reproduce the exact large distance physics of the problem. However, often they pick up the low lying manifold of excited states which becomes relevant at low enough temperatures. Also, 3-dimensional coupling in real materials helps to reduce the effect of fluctuations.

We consider here a minimal model with stripes to illustrate our conclusions. We employ the 2-dimensional one-band Hubbard Hamiltonian with hopping t and on-site repulsion U [2]. Superconductivity is introduced by including the nearest neighbor attraction V , which produces pairing predominantly in the d -wave channel close to half-filling [6]. The effective minimal Hamiltonian is thus

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle ij \rangle} n_i n_j, \quad (1)$$

where the operator $c_{i\sigma}^\dagger$ ($c_{j\sigma}$) creates (annihilates) an electron with spin σ on the lattice site i , and $n_i =$

$c_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger c_{i\downarrow}$ represents the electron density on site i . For our computations, we use the unrestricted mean-field approximation to this Hamiltonian,

$$H_{MF} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} \langle n_{i\downarrow} \rangle + \langle n_{i\uparrow} \rangle n_{i\downarrow} + \sum_{\langle ij \rangle} c_{i\downarrow} c_{j\uparrow} \Delta_{ij}^* + \text{H.c.}, \quad (2)$$

where $\Delta_{ij} = V \langle c_{i\downarrow} c_{j\uparrow} \rangle$ is the MF superconducting order parameter. The direct Hartree terms in V are neglected since the magnitude of the effective nearest neighbor attraction is expected to be much smaller than the on-site repulsion U . Hence, it should not affect the diagonal part of the Hamiltonian, which is responsible for the charge and spin order. Therefore, the effect of V in our model is limited to the generation of superconducting correlations. We do not address the very important issue of the microscopic origin of the attraction V . Our goal is only to construct a minimal model that may help to qualitatively understand the rich phase diagram of the cuprates. Unless stated otherwise, standard parameter values used are $U = 4t$ and $V = -0.9t$. This choice of parameters allows us to clearly demonstrate our conclusions regarding the inhomogeneous superconducting phase.

To self-consistently solve the MF equations we use an iterative scheme. This consists of two stages which are repeated until convergence is achieved: (1) Diagonalization of the MF Hamiltonian, and (2) Update of the MF parameters. An important feature of our approach is that all physical quantities are allowed to vary from one lattice site to another, e.g., $\langle n_{i\uparrow} \rangle \neq \langle n_{i\downarrow} \rangle$ and $\langle n_{i\sigma} \rangle \neq \langle n_{i+\alpha\sigma} \rangle$. Generically, we are seeking inhomogeneous solutions whose typical correlation lengths ξ involve several lattice spacings. Therefore, it is important that the simulated supercell size $N_x \times N_y$ (with periodic boundary conditions) is such that $N_{x,y} > \xi_{x,y}$. The Hamiltonian in Eq. (2) can be rewritten in the matrix form, $H_{MF} = \mathbf{c}^\dagger \hat{H} \mathbf{c}$, with $\mathbf{c} = (c_{1\uparrow}, c_{1\downarrow}, c_{2\uparrow}, c_{2\downarrow}, \dots)^T$,

where \hat{H} is a $(2N_x N_y) \times (2N_x N_y)$ hermitian matrix. By applying a unitary transformation α ($\alpha^{-1} = \alpha^*$) the Hamiltonian matrix can be diagonalized as $\hat{H} = \alpha \hat{D} \alpha^{-1}$, with $D_{nm} = \delta_{nm} E_n$. The Hamiltonian can be diagonalized in the Bogoliubov quasiparticles,

$$\gamma_n = \sum_m \alpha_{nm}^{-1} c_m, \quad (3)$$

with energies E_n . By reexpressing the original creation-annihilation operators in terms of the Bogoliubov quasiparticles, one can recompute the parameters of the MF Hamiltonian. For example,

$$\begin{aligned} \langle n_{i\uparrow} \rangle &= \langle c_{i\uparrow}^\dagger c_{i\uparrow} \rangle = \sum_{nm} \langle \alpha_{i\uparrow,n}^* \gamma_n^\dagger \alpha_{i\uparrow,m} \gamma_m \rangle \\ &= \sum_n |\alpha_{i\uparrow,n}|^2 n_F(E_n), \end{aligned} \quad (4)$$

where $n_F(E_n)$ is the Fermi-Dirac distribution function. Repeated until the convergence, the iterations produce the spatial profiles of the self-consistent density and order parameter.

A typical zero-temperature MF inhomogeneous solution is shown in Fig. 1. In the lowest energy configuration, the spin density develops a soliton-like AF anti-phase domain boundary — a stripe — at which the AF order parameter changes sign. At the domain boundary, the electronic charge density is depleted. The width of the domain wall, ξ_{DW} , decreases with increasing on-site repulsion U . However, for values of U that are not much larger than the hopping t , the charge per unit length of the optimal (the lowest energy) stripe remains the same and is close to unity near half-filling. This result, first demonstrated in this simple model by Schultz [2], is a direct consequence of doping-dependent nesting in the Hubbard model. The bond-centered stripes are favored relative to the site-centered ones, although the energy difference in our case is small due to the smooth charge distribution. For a different band structure the exact relation between the doping x and inter-stripe distance, $L(x)$, may change; however, any model whose ground state is AF at zero doping, is expected to have AF stripes for a finite doping, with incommensuration proportional to the doping, $1/L(x) \propto x$, near half-filling. For example, negative next-nearest neighbor hopping t' (relevant in the hole-doped cuprates [8]), modifies the stripe filling without compromising the stripe phase stability relative to commensurate AF at the MF level [7]. The stripe filling is a monotonically decreasing function of the magnitude of t' , with the magic filling 1/2 occurring when $t' = -0.35t$. Experimentally, however, the value of the effective doping-dependent t' is still not well defined. Among the consequences of the doping dependence of t' are doping-dependent stripe filling, and a possibility of a transition from vertical to diagonal stripes as a function of doping. While we focus here on the model case $t' = 0$,

our conclusions remain qualitatively the same also in the presence of a moderate negative $|t'| \lesssim 0.5t$.

For large enough doping levels, such that $L(x) \lesssim \xi_{DW}$, the AF stripes begin to overlap. In this regime the excitation spectrum is no longer fully gapped and mobile carriers appear. Further doping mostly changes the amplitude of the spin and charge density waves, only slowly modifying the incommensuration, $1/L(x)$ [2]. When the stripes are sufficiently close to melting, the AF aspect of the problem becomes unimportant, and the superconductivity is of the conventional BCS type.

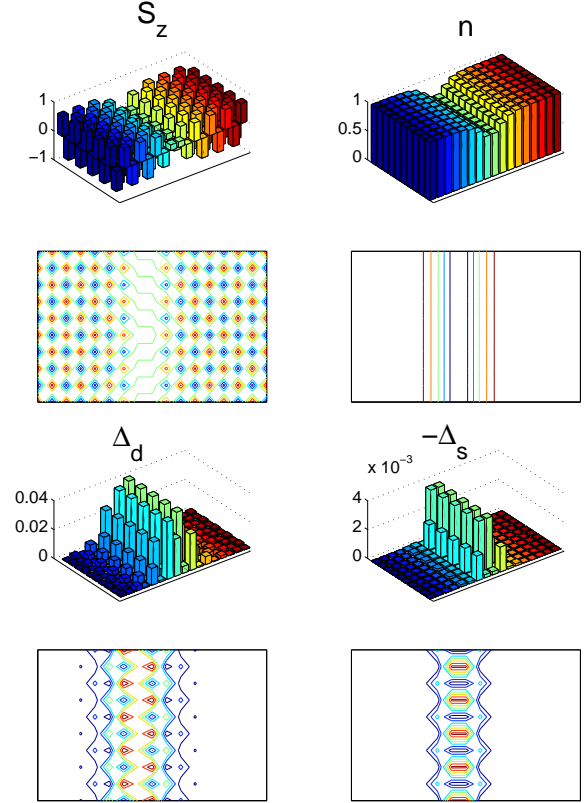


FIG. 1. Typical example of density and superconducting order parameter profiles in a stripe state (here period 17). The top two bar charts represent the site-dependent spin and charge densities, respectively. The contour plots indicate the sites with low (blue) and high (red) values of the corresponding densities. The bottom four plots show the values of the superconducting order parameters, defined as $\Delta_i^{d(s^*)} = (\Delta_{i,right} + \Delta_{i,left} \mp \Delta_{i,up} \mp \Delta_{i,down})/4$ for d -wave (extended s -wave) order parameter on site i ($U = 4t$, $V = -0.9t$). Different choices of parameters lead to qualitatively similar patterns, with stronger U leading to a stronger AF order and more attractive V causing the superconducting stripes to become wider and larger in amplitude. The doping level is 5.9%.

The superconducting order parameter $\Delta_{ij}^{d(s^*)}$ is maximal on the stripes and is not smooth (even within the stripe) due to the presence of the AF background. This

happens since the order parameter is sensitive to the spin density on sites i and j . If i belongs to the spin-down sublattice and the neighbor j is on the spin-up sublattice, then the order parameter is large, and vice versa. Notice, that in addition to the dominant d -wave component, there is a small extended s -wave component generated on the stripe, which can be interpreted as a distortion of the d -wave at the level of about 10%. This happens because a symmetry of the lattice has been broken. The superconducting stripe is pinned by the AF phase domain boundary. Since the spin density on the domain boundary is small, a natural interpretation is that the superconductivity is suppressed in the regions of large AF order. Nevertheless, the width of a superconducting stripe, ξ_{SC} , is determined not only by the width of the AF stripe, but also increases rapidly with increasing magnitude of the nearest neighbor attraction, V . For our choice of parameters, $\xi_{DW} \sim 4$ and $\xi_{SC} \sim 8$ lattice sites. For dopings smaller than about 10% (corresponding to $L(x) > 10$ lattice sites) the stripes have negligible overlap. In this regime, the amplitude of the superconducting order parameter on the stripes no longer depends upon the stripe-stripe separation. For higher doping levels, an overlap between the superconducting order parameters on adjacent stripes is established.

A central question is connected to the conducting properties of the resulting inhomogeneous state: Is it a global superconductor, a metal, an insulator, or some unusual anisotropic phase? To resolve this issue we use the concepts of charge stiffness D_c [9], which measures the sensitivity of the ground state to changes in boundary conditions, and anomalous flux quantization [10], which provides a direct signature of the Meissner effect. These concepts, together with topological quantum numbers [11], are routinely employed to study the localization properties of models of interacting electrons. To compute D_c one needs to determine how the energy of a system with a fixed number of particles, E , depends on the twist in the boundary conditions, $\Theta \in [0, 2\pi)$. The twist of the boundary conditions is independently applied along each spatial direction $j = x, y$ and implies that $c_{N_j+1} = \exp(i\Theta)c_1$. The special case of $\Theta = 0$ corresponds to strictly periodic boundary conditions. Textbook schematics of the energy dependence, $E(\Theta)$, are shown in Fig. 2A. The calculated many-particle spectrum $E(\Theta)$ for a system with a stripe separation of 17 lattice sites in our model is shown in Fig. 2B. The energy curves imply that the system is superconducting, however the superfluid stiffnesses along and across the stripes are drastically different. However, for a smaller stripe periodicity (Fig. 2C), due to substantial overlap between the stripes, superconductivity is almost as strong across the stripes as it is along the stripes.

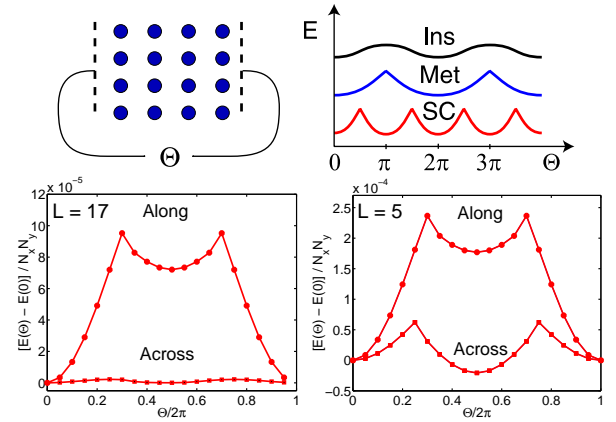


FIG. 2. (A) Schematics of typical energy spectra, $E(\Theta)$. Insulating behavior is characterized by a smooth curve of period 2π , with an amplitude that decays exponentially with system size. The metallic and the superconducting states typically have patterns with cusps, with variations in $E(\Theta)$ that decrease as a power of the system size in such a way that the charge stiffness, $D_c = \frac{L}{2} \partial^2 E / \partial \Theta^2$, remains constant. The superconducting behavior is distinguished from the metallic one by the reduced periodicity, referred to as anomalous flux quantization (AFQ). There is a direct correspondence between AFQ and the fact that the minimum flux that can penetrate a superconducting system is one half of the flux quantum, $\phi_0/2 = \hbar c/2e$. The exact period π is only achieved in the thermodynamic limit; for a finite system, there is only a signature of the reduced period. (B) Calculated energy spectrum $E(\Theta)$ for a system of size 10×17 (see Fig. 1). Along the stripes there is a pronounced AFQ signature, which implies that the system is superconducting along the stripes. The energies were computed at a fixed chemical potential. To convert to the energy at a fixed average number of particles, a density adjustment by the amount $-\mu(n(\Theta) - n(0))$ has been made. Across the stripes, the stiffness is very small, but has a period of π . Hence the system appears to be a global superconductor, but with an extremely small superfluid stiffness in the direction across the stripes. (C) Calculated energy spectrum $E(\Theta)$ for a system of size 10×15 with 3 stripes of period 5. Due to substantial overlap between the superconducting stripes, this system has superconducting strengths that are comparable in both directions.

Arrays of superconductors separated by insulating regions, known as Josephson junction arrays, have non-trivial conducting properties. Depending on the relative strength of the coupling between the superconductors and the charging energy, such systems can be either superconductors or insulators [12]. At the MF level, the charging aspect of the problem is absent, and hence we can expect a global superconductor at zero temperature no matter how weak the interchain coupling is. In a real system, for a sufficiently weak coupling the superconducting behavior will be suppressed. In the case of superconducting channels separated by AF insulators, the coupling is inversely related to $L(x)$. For very large

$L(x)$ at low doping, $L(x) \gg \xi_{SC}$, the overlap between the superconducting stripes, and hence the superconducting transition temperature T_c , is exponentially small. As the distance between the stripes decreases (larger doping), the overlap of the superconducting condensate wave functions should establish a phase coherent superconducting state. Indeed, this is qualitatively what we observe already at the mean-field level in the striped superconductors. For a large superconducting stripe overlap, the effective coupling between the stripes is non-exponential. In this regime, the experimentally measured superconducting transition temperature is proportional to incommensuration [13], which implies that the effective Josephson coupling scales as $1/L(x)$.

A possible experimental test of the Josephson-coupled superconductor scenario proposed here (see also [14]) can be performed by measuring the in-plane Josephson plasmon resonance. The resonance should be present in the microwave-frequency range and is excitable by an in-plane electric field.

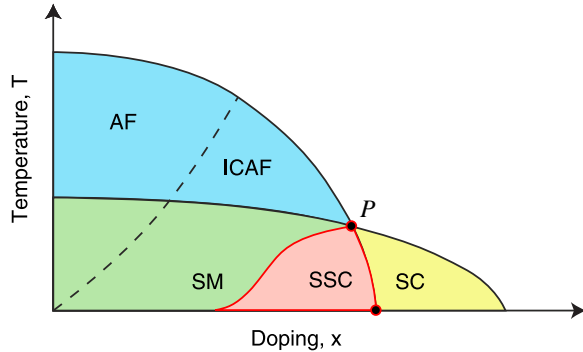


FIG. 3. Schematic phase diagram obtained by superimposing the antiferromagnetic (AF) / striped (ICAf) and the d -wave superconducting (SC) phase diagrams. In the intersection region we distinguish the subregions of Josephson-coupled striped superconductor (SSC), and non-superconducting “strange metal” (SM), which is neither a superconductor, nor a simple insulator. The upper boundary of the AF/ICAf corresponds to the weak pseudogap crossover, and the line between the pure AF/ICAf and the SM marks the strong pseudogap crossover. In the very low doping region, the superconducting aspect of the problem becomes irrelevant, and the phase diagram is dominated by the physics of antiferromagnets. A detailed finite-temperature study is required to precisely locate the left boundary of the SSC region, and hence to determine if the critical point P is indeed a penta-critical point.

From our zero-temperature analysis of the coexistence of AF stripes (ICAf) and superconductivity, a simple qualitative thermodynamic phase diagram emerges. In the conjectured phase diagram, we utilize the finite-temperature AF/ICAf phase diagram of the Hubbard model together with the superconducting (SC) phase di-

agram of the t - V model. The SC phase diagram is obtained in the homogeneous MF [6], while the AF/ICAf phase boundary is constructed under the assumption of the second order phase transition between the homogeneous and inhomogeneous states [2]. For a suitable choice of parameters, for instance $U = 2t$ and $V = -t$, the SC and the AF/ICAf regions in the phase diagram intersect, as shown in Fig. 3. The boundary between the AF and ICAf phases corresponds to an infinite period stripe modulation, and implies that the incommensuration is a decreasing function of temperature. The energy scale associated with the AF/ICAf region of the phase diagram is much larger than that of the SC part. Thus, one expects that only the SC phase boundary is modified when it passes through the AF/ICAf region. The central result of our work is that the superconductivity *does not* disappear in the region of the AF stripes, but rather becomes striped, with anisotropic superfluid stiffness.

Based on familiar Josephson coupling physics, in the region of coexistence of superconductivity and stripes, we can expect a part that is a globally coherent striped superconductor (SSC). The rest of the intersection region is covered by an exotic phase which, if it were perfectly orientationally ordered, would be a superconductor in one direction and a strongly-correlated insulator in the other. In reality, due to the meandering of the stripes and their break-up into finite segments [15], the state is likely to be highly inhomogeneous and neither an insulator, nor a superconductor, but also not a simple metal. In agreement with the experimental attribution, we refer to this region as a “strange metal” (SM). The line separating the SM from the AF/ICAf region, in the context of the experiments, can be associated with the crossover to the strong pseudogap regime, and corresponds to the opening of the superconducting gap. The high-temperature AF/ICAf phase boundary marks to onset of the weak pseudogap. For very small dopings the MF stripe separation becomes so large that the superconducting aspects of the model become irrelevant and one crosses over to the regime governed predominantly by the physics of antiferromagnets.

It should be emphasized that the phase diagram presented here is based on the (inhomogeneous) MF treatment of a 2-dimensional model. As such, it is susceptible to the quantum and thermal fluctuations that tend to destroy long-range order. For instance, the ICAf phase in Figure 3 in a real material is more likely to manifest itself as incommensurate AF fluctuations, rather than a pure phase. However, the effects of the 3rd dimension and impurity pinning may stabilize the MF phases at a sufficiently low temperatures, revalidating the MF phase diagram.

Within our model, we find that increasing on-site repulsion leads to a suppression of superconductivity. For larger U , the pure d -wave superconducting region of the phase diagram (SC) shrinks, and the width of the superconducting stripes in the SSC region decreases. For

example, changing U from $4t$ to $5t$ (keeping V fixed) leads to a five-fold reduction of the superconducting order parameter on stripes. This is in contrast with the *homogeneous* mean-field results [6], there the d-wave superconductivity is independent of the magnitude of U . On the other hand, large values of the on-site repulsion, $U > 4t$, in the Hubbard model lead to *diagonal* stripes [16]. Applying our model to diagonal stripes ($U = 5t$, $V = -0.9t$), we find that superconductivity vanishes completely at the optimal stripe filling. Perhaps it is not a coincidence, that the insulating cuprates do in fact show diagonal stripes, as opposed to the lattice-aligned stripes in the superconducting cuprates [17].

There is an analogy between the role played by doping in our model, and the strength of the electron-phonon coupling, λ , in the McMillan criterion for the maximum achievable T_c in conventional superconductors [18]. In McMillan's picture, increasing λ favors superconductivity. However, increasing λ too much induces a structural transition, and hence changes the reference ground state. In our model, increasing doping brings the superconducting stripes closer together, and hence enhances the global T_c . However, increasing doping too much causes a transition to the uniform state, with a subsequent monotonically decreasing T_c as a function of doping.

The topology of the phase diagram we have proposed appears to be relevant for the superconducting cuprates, such as LSCO and YBCO. The same simple model (for other parameter values) can produce other topologies as well. A non-trivial topology, which may be realized in a material with a weaker attractive coupling, is when the superconducting region is fully contained in the AF/ICAF region. Depending on the parameters, such a material may be a striped superconductor in a certain range of dopings. Also, similar physics may occur in organic charge-transfer salts [19], that show AF, ICAF and superconductivity under pressure which controls inter-chain coupling. There, the intrinsically anisotropic coupling is also important for the stabilization of the mesoscopic inhomogeneities [20].

In conclusion, we find that a simple one-band model with on-site repulsion and nearest-neighbor attraction, in an appropriate range of parameters, can simultaneously sustain both incommensurate antiferromagnetism and inhomogeneous superconductivity. Prompted by this finding and utilizing well-known antiferromagnetic and superconducting phase diagrams, we have constructed a generic phase diagram that captures many of the phases

observed in the cuprate and organic superconductors. An experimental test of the Josephson-coupled superconductor proposed here (see also [14]) can be performed by measuring the in-plane Josephson plasmon resonance. Although our simple model appears to capture much of the observed rich physics, however it can be readily elaborated (with multiple electron bands, 3-dimensionality, long-range interactions, lattice coupling, etc.) for more quantitative comparisons with specific materials.

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